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A LINK BETWEEN THE PHENOMENOLOGICAL AND PHYSICAL MODELLING OF TRANSFORMATION-INDUCED PLASTICITY

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Abstract. In high temperature shape memory alloys, the inelastic deformation mechanism is a combination of the transformation strain, viscoplastic strain in austenitic and martensitic phases, and transformation-induced plasticity. The latter is a consequence of the effect of austenite↔martensite transformation on the dislocation dynamics. In this study, the effect of the martensitic plates in microstructure, in the case of the internal stress field, is shown by a theoretical solution of the martensitic inclusions. The one-dimensional phenomenological continuum model is presented to predict the macroscopic behavior of a sample high temperature shape memory alloy by making a link between the internal stress field of the microstructure and the phenomenological model.

1 INTRODUCTION

High temperature shape memory alloys (HTSMAs) are shape memory alloys with higher transformation temperatures (TT), usually above 100°C. Similar to other shape memory alloys (SMAs), two way shape memory effect and pseudoelasticity are the most two significant behavior of HTSMAs at high temperatures. These behaviors come from the diffusionless solid-solid martensitic transformation between austenite and martensite phases under thermo mechanical loadings. To apply the HTSMAs in the industry (especially as a high temperature actuator), they have to show acceptable recoverable transformation strain, long term stability and resistance to the plastic deformation in both austenite and martensite phases during the martensitic transformation to avoid occurrence of the irrecoverable strains during their performance [1].

The irrecoverable plastic strain in HTSMAs during thermomechanical cycling is supposed to be due to the dislocation glides in the austenite phase, detwining and reorientation of martensitic variants in the martensite phase, and retained martensitic phases in the microsturcture. Furthermore, in some cases, the transformation induced plasticity may be an effective deformation mechanism in the shape memory alloys [2], because the transformation strain in these alloys affects the value of the internal stresses and enhances the dislocation gliding in austenite phase, such as what happens in the TRIP steels [3].

In this work, to investigate the effective parameters of transformation-induced plasticity in SMAs, the microstructure of a austenitic/martensitic domain at a specific time during phase transformation is studied. Then the changes of the internal stress field due to the existence of the martensitic region inside the austentitic medium are investigated by using the solution for an eigen-strain problem [4, 5], with the consideration of the elliptical martensitic inclusions in a plane strain problem. The results show the increase in the internal stress fields of microstructure which may enhance the dislocation dynamic in the austenitic phase and named as transformation induced plasticity [3].

Recently some experiments are done on the $TiPdNi$ HTSMAs and the coexistence of the transformation strain and the irrecoverable plastic strains is observed [6, 7]. Some researchers also presented macroscopic constitutive models for predicting the behavior of HTSMAs under thermomechanical loadings [8]. Although it is important to model the coexistance of martensitic transformation and viscoplasticity at high temperatures, it is still inevitable to investigate the role of the transformation induced plasticity during the martensitic transformation. As a result, a one dimensional constitutive model based on the isotropic plasticity consideration is presented to model the thermomechanical behavior of HTSMAs. The phenomenological kinetic equation is suggested by [9] to predict the transformation induced plastic strain during the austenite$\leftrightarrow$ martensite transformation under external applied stress. The results obtained from the micro-structural model support the phenomenological model for transformation-induced plasticity.

Thus, the main objectives of this work are: (1) develop a microstructral model of the martensite plates in austenitic matrix based on the theory of inclusions and eigenstrains during martensitic transformation; (2) develop a one-dimensional phenomenological continuum model of high temperature shape memory alloy to model the transformation induced plasticity; (3) compare the results of thermal cycling uniaxial experiments to show the availability of the constitutive equations.

The structure of this paper is as follow. In Section 2, the description of the model and the theoretical formulation of the stress field of martensitic inclusions in austenitic matrix are presented. The results of implementation of theoretical solution and discussion about the effect of the martensitic plate on the internal stress field of microstructure are presented in Section 3. In Section 4 a one-dimensional phenomenological continuum

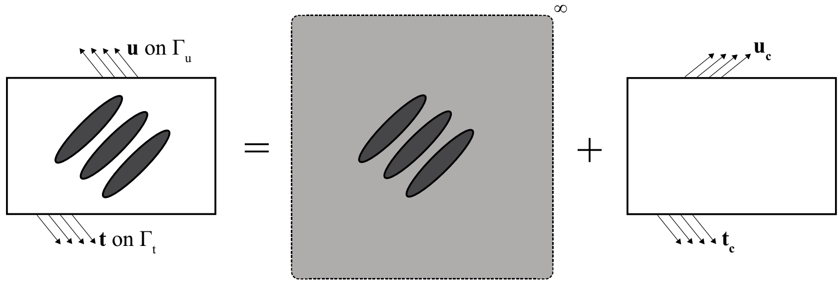


Figure 1: Decomposition of the problem to an inclusion problem and a complementary case

model based on the results of previous section is presented to model the thermomechanical behavior of high temperature shape memory alloys. Finally, the conclusions of this study are discussed in Section 5.

2 MODEL DESCRIPTION AND FORMULATION

2.1 Model assumptions

To study the effect of martensitic regions in asutenitic matrix, the following assumptions are considered. A linear elastic body of volume V with boundary ∂V including linear elastic martensitic inclusions of volume V^m is considered as the framework. The fourth-order elastic moduli of the austenite and the martensite regions are assumed to be $\mathcal{C}^a$ and $\mathcal{C}^m$ accordingly. The cell is under periodic boundary condition with loading of macroscopic average strain tensor $\bar{\boldsymbol{\epsilon}}$. It is also assumed that the loading is applied quasi-statically and the model is the solution of the equilibrium problem of the specimen at a selected time. To investigate the effect of martensitic inclusion, the model is a superposition of two problems as shown in **Figure** 1.

As shown in **Figure** 1, the total problem decomposes to two sub-problems: (i) martensitic inclusions in infinite medium, (ii) a complementary problem in finite austentitic region to satisfy the boundary conditions of the total problem. The decomposition for stress, strain and displacement fields may be written in following form:

$$\begin{aligned} \mathbf{u} &= \mathbf{u}^m + \mathbf{u}^c \\ \boldsymbol{\sigma} &= \boldsymbol{\sigma}^m + \boldsymbol{\sigma}^c \\ \boldsymbol{\varepsilon} &= \boldsymbol{\varepsilon}^m + \boldsymbol{\varepsilon}^c \end{aligned} \tag{1}$$

where $\mathbf{u}^m$, $\boldsymbol{\sigma}^m$ and $\boldsymbol{\varepsilon}^m$ are displacement, stress and strain fields of the infinite domain of austenite with the martensitic inclusions and $\mathbf{u}^c$, $\boldsymbol{\sigma}^c$ and $\boldsymbol{\varepsilon}^c$ are displacement, stress and strain fields of the finite complementary problem. The summation of these two cases gives the total problem with displacement and traction on the boundary according to the loading conditions. Here, the nucleation and growth of the martensitic plates and the dislocation dynamics are not the aim of study; however, the stress, strain and displacement

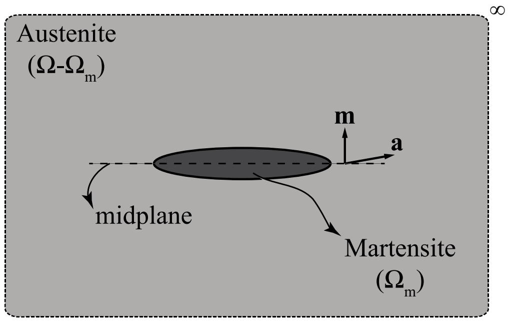


Figure 2: Schematic of two dimensional plane strain region including the martensitic plate in local cordinates

fields of martensitic regions in austenitic matrix at a selected time is important for us to investigate the effect of the martesitic phase on the total state of the region.

2.2 Stress-field due to the martensitic region

In this problem we consider the martensitic phase transformation for TiPdNi High temperature shape memory alloy that has cubic structure in austenite and orthorhombic structure in the martensite state. Solving the crystallographic model of the martensitic transformation by applying the minimization method [10], the 96 possible transformation systems for austenite-twin martensite were found. Each of these crystallographical systems consist of a pair of vectors $(\mathbf{a}, \mathbf{m})$, where $\mathbf{m}$ is the habit plane normal vector and $\mathbf{a}$ is the transformation shape vector. In this study we consider that the calculated crystallograpics are the same for constrained and unconstrained condition of twin martensite.

The transformation strain tensor of a specific transformation system is combined from the simple shear ($\gamma = \mathbf{a}.\mathbf{m}$) and the volumetric expansion ($\delta = \sqrt{|\mathbf{a}|^2 - \gamma^2}$) which can be expressed as equation (2).

$$\varepsilon^{tr} = \frac{1}{2}\left(\mathbf{a} \otimes \mathbf{m} + \mathbf{m} \otimes \mathbf{a}\right) \tag{2}$$

In this study, the two dimensional plane strain problem is modeled and only one of the 96 transformation systems is considered. Therefore, the simulation coordinates has been rotated until the habit plane normal be in local y direction. This consideration is based on our goal to simulate the effect of a martensitic region on the internal stress field of the specimen. **Figure** 2 shows the schematic of the two dimensional plane strain model and the shape of a martensitic transformation plate.

As indicated in previous section, the stress field of the martensitic plates is calculated in infinite domain where the martensitic regions play the inclusion role with an eigen-strain. This is a function of uniform transformation strain inside the martensitic region and the inhomogeneity of austenite and martensite phases. The stress, strain and displacement fields of martensitic inclusion in this study are presented by theoretical solution for elliptical cylinder inclusion for interior and exterior points in the infinite domain under plane strain.

Eshelby [11] proved that the strain and stress fields inside the inclusion are uniform, and Mura [4] showed the relation between strain field inside the inclusion and the eigenstrain as given in equation (3).

$$\varepsilon_{ij} = \mathrm{S}_{ijkl}\varepsilon^{\star}_{kl} \tag{3}$$

Here, S_{ijkl} is called the Eshelby tensor that is constant inside the inclusion, and $\boldsymbol{\varepsilon}^{\star}$ is the eigenstrain tensor. For the martensitic inclusion problem, $\boldsymbol{\varepsilon}^{\star}$ is given by equation (4).

$$\boldsymbol{\varepsilon}^{\star} = [(\mathrm{C}^{m} - \mathrm{C}^{a})\mathrm{S} + \mathrm{C}^{a}]^{-1}\mathrm{C}^{m}\varepsilon^{tr} \tag{4}$$

From the strain field, the stress field for interior points is expressed by equation (5).

$$\sigma_{ij} = \mathrm{C}^{m}_{ijkl}\varepsilon_{kl} \tag{5}$$

For the exterior points:

$$\begin{aligned} \varepsilon_{ij} &= \mathrm{D}_{ijkl}\,(x)\,\varepsilon^{\star}_{kl} \\ \sigma_{ij} &= \mathrm{C}^{m}_{ijkl}\varepsilon_{kl} \end{aligned} \tag{6}$$

where $\mathrm{D}\,(x)$ is the Eshelby tensor for exterior points that relates the strain field to eigenstrain, and it is a function of the position of the exterior points. For brevity the derivation of Eshelby tensor(for interior and exterior points) and displacement fields are not present here; one can obtain the close form solution based on [4].

Finally, after the implementation of the theoretical solution for stress, strain and displacement field of each inclusion in infinite body, a summation is done in the entire specimen for different martensitic plates.

2.3 Stress-field of complementary problem

The complementary problem is used to satisfy the boundary conditions of the original problem. The problem is in finite domain and the boundaries can be defined based on (2) :

$$\begin{aligned} \mathbf{u}^{c} &= \mathbf{u} - \mathbf{u}^{m} \qquad \mathit{on}\ \Gamma_{u} \\ \mathbf{t}^{c} &= \mathbf{t} - \mathbf{t}^{m} \qquad \mathit{on}\ \Gamma_{t} \end{aligned} \tag{7}$$

where $\mathbf{t}$ is traction vector, and Γ_u and Γ_t are the displacement and the traction boundaries. Therefore, the boundary conditions of complementary problem are defined after solving the inclusion problem.

The finite element method is applied to solved the complementary problem. A finite element code is written with the consideration of periodic boundary conditions.

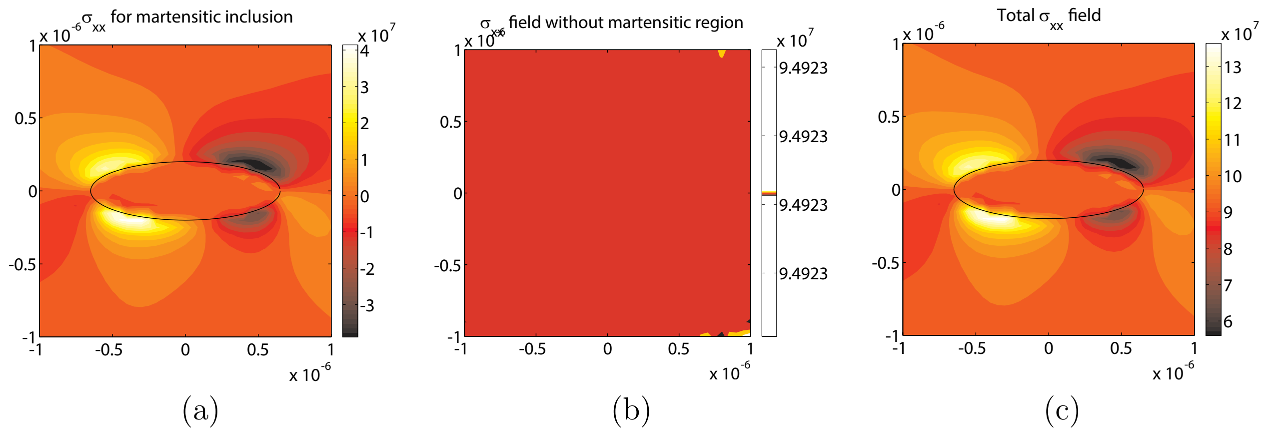


Figure 3: σ_{xx} field for (a) martensitic inclusion in infinite medium, (b) complementary problem without martensitic region and (c) total problem

3 RESULTS AND DISCUSSIONS

3.1 Effect of martensitic inclusion on internal stress field in specimen

In this section a large martensitic plate is considered in the domain and the σ_{xx} stress field (the stress in x direction which is the direction of uniaxial loading in this problem) for three cases: (i) just the martensitic inclusion, (ii) complementary problem and (iii) the superposition of them (total problem) are shown in **Figure** 3.

As can be seen in **Figure** 3b and 3c, the total stress field in a problem considering the martensitic inclusion is higher in some regions than the problem without considering the martensitic plate. It clearly shows that the actual stresses in the domain that affect the deformation mechanism at each time is different from the stresses due to just external loading. It is clear in **Figure** 3b that the stress field of the complementary problem with above boundary condition is uniform in the entire domain.

In the next step, a numbers of martensitic inclusions with the same transformation variants are considered in the model. The stress field of this array of transformation inclusions is illustrated in **Figure** 4.

As can be seen in **Figure** 4, by increasing the numbers of transformation plates in a domain, the areas which their stress field is affected by martensitic inclusions are increased. Therefore the effect of martensite phase on internal stress of the domain is more significant.

Th martensite volume fraction is defined by the ratio of the volume of the martensitic regions to the total volume of the domain and it is computed by (8)

$$\zeta^m = \frac{1}{\Omega} \sum_{1}^{N^m} \Omega_k^m \tag{8}$$

It is now clear that by changing the martensitic volume fraction the internal stress field is changing and from the comparison of **Figures** 4a , 4b and 4c that increasing the ζ^m will increase the areas with the higher internal stress than the external stress.

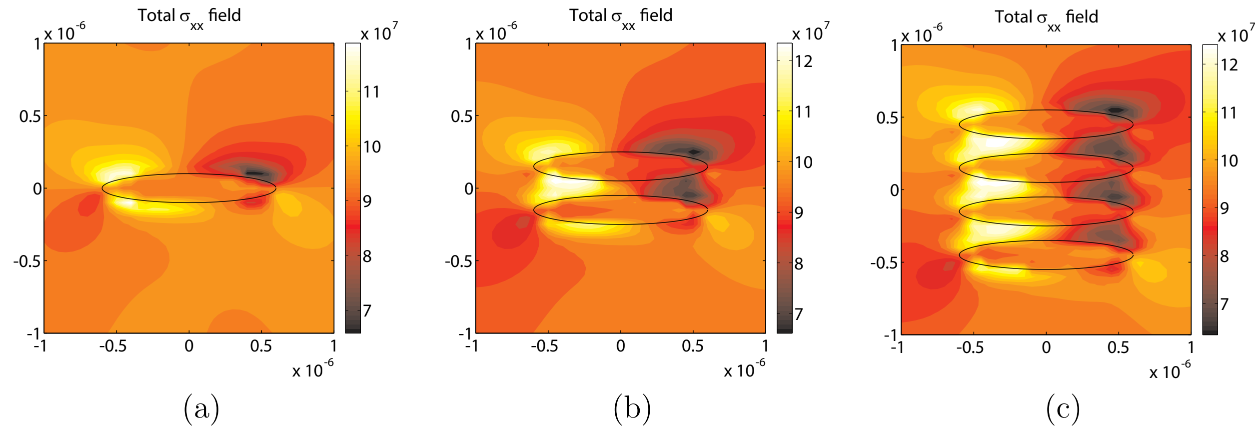


Figure 4: Total σ_{xx} field for (a) one martensitic plate, (b) two martensitic plates and (c) four martensitic plates

3.2 Effect of crystallographic transformation systems on stress field

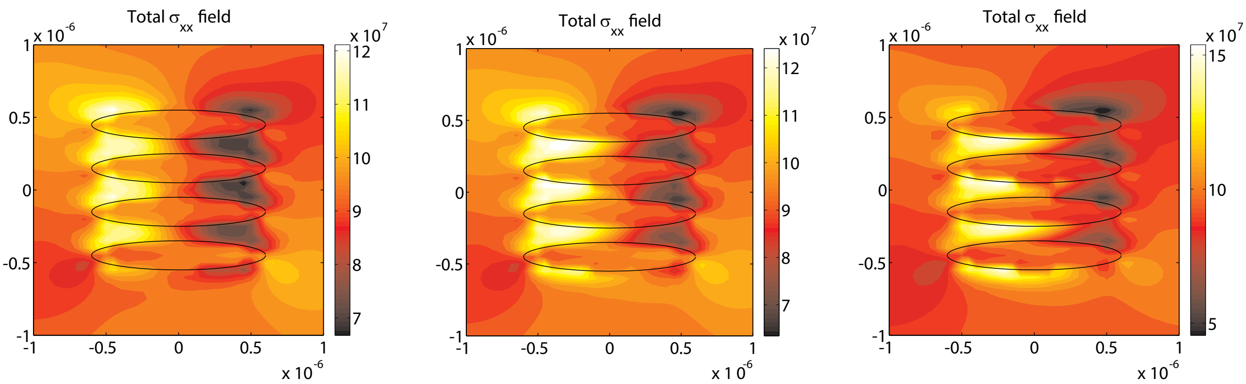
To study the effects of crystallogeraphic systems for transformation, the model is repeated with transformation systems of NiTi shape memory alloy and for TRIP steel. For each of them, one of the transformation systems is considered as presented in **Table** 1, and then the local stress field of each one in the plane strain problem is obtained.

Table 1: Different transformation systems for different materials

Alloy	**a**	**m**
$NiTi$	(0.0375,-0.1008,0.0278)	(0.4565,-0.04197,-0.8887)
$Ti_{50}Pd_{40}Ni_{10}$	(0.0902,0.0787,-0.0342)	(0.6723,-0.7176,-0.1817)
Trip *Steel*	(-0.0345,0.1142,-0.1360)	(0.1711,-0.5666,-0.8060)

The internal stress field for these materials under the same external loading are presented in **Figure** 5.

By comparing the **Figures** 5a, 5b and 5c for $NiTi$, $Ti_{50}Pd_{40}Ni_{10}$ shape memory alloys and TRIP steel and paying attention to the magnitude of transformation strain, it can be concluded that the transformation strains have special effect on the internal stress field of the domain and the bigger transformation strain, which depends on the crystallographic configuration, gives higher stress inside the domain.



(a) (b) (c)

Figure 5: Total σ_{xx} field for (a) $NiTi$, (b) $Ti_{50}Pd_{40}Ni_{10}$ and (c) steel

4 LINK THE MICROSTRUCTURE MODELING WITH CONTINUUM MODELING

In this section, a phenomenological one-dimensional continuum model for the high temperature shape memory is presented based on the qualitatively study that is done on the microstructure of martensitic plates and the transformation in the previous sections. As it is illustrated, with the existence of martensitic plates, the martensitic volume fraction and the magnitude of the crystallographically transformation strain affect the microstructural stress field, which is important in the deformation mechanisms. According to these results, the driving force for inelastic deformation mechanism, such as transformation and dislocation dynamic, should be calculated according to the internal stresses, which are in some cases much different from stresses due to the external loadings.

The governing variable in the constitutive model are taken as: (i) the applied external stress, σ; (ii) total strain, ε; (iii) elastic strain, ε^e; (iv) inelastic strain ε^{inel}; (v) absolute temperature, θ; (vi) total martensite volume fraction, ξ; with $0 \leq \xi \leq 1$.

To develop the one dimensional isotropic based constitutive equations, one may consider that the total value of strain is a combination of the elastic and the inelastic parts:

$$\varepsilon = \varepsilon^e + \varepsilon^{inel} \tag{9}$$

where ε^e is the thermo-elastic strain and ε^{inel} is the inelastic part of strain due to the transformation, plasticity in both phases and transformation-induced plasticity. For the first term it is clear to have:

$$\varepsilon^e = \frac{1}{E}\sigma + \alpha\left(\theta - \theta_0\right) \tag{10}$$

where α is the thermal expansion coefficient, θ_0 is the reference absolute temperature and E is the elastic module of the austenite or the martensite phases. The inelastic part of strain is combined of four parts as below:

$$\dot{\varepsilon}^{inel} = \dot{\varepsilon}^t + (1-\xi)\dot{\varepsilon}_A^{vp} + (\xi)\dot{\varepsilon}_M^{vp} + \dot{\varepsilon}^{tp} \tag{11}$$

where $\dot{\varepsilon}^t$ is the transformation strain rate, $\dot{\varepsilon}_A^{vp}$ and $\dot{\varepsilon}_M^{vp}$ are the plastic strain rate in the austenite and the martensite, $\dot{\varepsilon}^{tp}$ is the transformation-induced plastic strain rate and ξ is the martensitic volume fraction.

Transformation strain occurs during the martensitic transformation due to the change in the crystalline structures from the austenite (higher symmetry) to the martensite (lower symmetry). This strain begins when austenite phase starts to transform to martensite and it stops when all the domain transforms to the martensite. The same happens during the backward transformation from the martensite to the austenite. Therefore, the transformation strain rate should be a function of the martensitic volume fraction and a material parameter comes from crystalline structure:

$$\dot{\varepsilon}^t = sgn(\sigma)\varepsilon^{tr}\dot{\xi} \tag{12}$$

where ε^{tr} is the magnitude of the microstructural martensitic transformation strain. To model the generation of new phase a power law kinetic equation is suggested for martensitic volume fraction:

$$\dot{\xi} = sign\left(f\right)\dot{\xi}_0\left(\frac{|f|}{f_c}\right)^{\frac{1}{m}} \tag{13}$$

where m is the *rate sensitivity* factor for the phase transformation (which is a small value for the rate independent mechanism), $\dot{\xi}_0 > 0$ is the *reference martensite or austenite generation rate*, f is the driving force for martensitic transformation and f_c is the material resistance to the transformation.

The driving force for martensitic transformation is a thermo-mechanical force which can be found from:

$$f = |\sigma|\,\bar{\varepsilon}^t - \frac{\lambda_T}{\theta_T}\left(\theta - \theta_T\right) - h\xi \tag{14}$$

where λ_T is the latent heat of the phase transformation, h is the transformation hardening factor due to the interactions between different phases and θ_T is the transformation temperature define as:

$$\theta_T = \frac{M_s + A_s}{2} \tag{15}$$

where M_s and A_s are the martensite start and the austenite start temperatures, respectively.

Due to the high transformation temperatures (0.3-0.5 melting temperature) and activation of the creep mechanisms, the rate-dependent kinetic equations for the plastic strain rate in the austenite and the martensite phases are suggested as:

$$\begin{cases} \dot{\bar{\varepsilon}}_A^p = \dot{\varepsilon}_0 sign\left(\overline{\tau}\right)\left(\frac{\overline{\tau}}{S_a}\right)^{\frac{1}{n}} exp\left(\frac{-Q_a}{R\theta}\right) \\ \dot{\bar{\varepsilon}}_M^p = \dot{\varepsilon}_0 sign\left(\overline{\tau}\right)\left(\frac{\overline{\tau}}{S_m}\right)^{\frac{1}{n}} exp\left(\frac{-Q_m}{R\theta}\right) \end{cases} \tag{16}$$

where n is the *rate sensitivity* factor, $\dot{\varepsilon}_0$ is the *reference strain rate*, Q_A and Q_M are the activation energy for austenite and martensite and R is the Stefan-Boltzmann constant and S_a and S_m are the plasticity resistance in austenite and martensite phases.

The phenomenological kinetic equation to predict the transformation induced plasticity is suggested by [9] as below:

$$\dot{\bar{\varepsilon}}^{tp} = \dot{\varepsilon}_0^{tp} \left(\frac{\overline{\tau}}{S_a} \right) \tag{17}$$

$$\dot{\varepsilon}_0^{tp} = \delta \dot{\phi} \left(\xi \right) g \left(\overline{\tau} \right) \tag{18}$$

where δ is the volumetric change of crystals between austenite and martensite phases that is found by microstructure calculation on crystals. $\phi \left(\xi \right)$ is a function of the martensitic volume fraction which increase from zero to one during transformation from the austenite to the martensite and is assumed as $\phi \left(\xi \right) = \xi \left(1 - \ln \xi \right)$, and $g \left(\overline{\tau} \right)$ is a function to describe the nonlinearity of relation between $\dot{\varepsilon}_0^{tp}$ and $\overline{\tau}$ and is suggested by [9] as

$$g \left(\overline{\tau} \right) = \begin{cases} 1 \quad if \quad \frac{\overline{\tau}}{S_a} < \frac{1}{2} \\ 1 + a \left(\frac{\overline{\tau}}{S_a} - \frac{1}{2} \right) \quad if \quad \frac{\overline{\tau}}{S_a} > \frac{1}{2} \end{cases} \tag{19}$$

Therefore, the final kinematic relation for the plastic (irrecoverable) strain is as below:

$$\dot{\bar{\varepsilon}}^{p}_{total} = (1 - \xi) \dot{\bar{\varepsilon}}^{p}_{A} + (\xi) \dot{\bar{\varepsilon}}^{p}_{M} + \dot{\bar{\varepsilon}}^{tp} \tag{20}$$

The one-dimensional isotropic-plasticity-based constitutive equations are implemented in a MATLAB code by developing a time integration algorithm, then the constitutive parameters are calibrated for $Ti_{50}Pd_{40}Ni_{10}$ high temperature shape memory alloy and then the one dimensional thermal cycling problem under external loading solved for different temperature rates and different external loads. The simulation are performed for thermal cycling between 520°C and 300°C (which this range includes the transformation temperatures) with two temperature rates of $2°C/min$ and $20°C/min$ under 100MPa and 200MPa external applied stress. Then the results are compared with thermal cycling experiments which were done by [6] and the comparisons are presented in **Figure** 6.

As can be seen in **Figure** 6, there is a good agreement between the values predicted by the phenomenological models and the experiments. The **Figures** 6 illustrates that although the temperature rate is high in these tests ($20°C/min$), and as a result, the value of rate dependent palstic strain is small, there is still some irrecoverable strain. This is because of the transformation induced plasticity (TRIP) in the high temperature shape memory alloy.

TRIP strain is not very common in most of the shape memory alloys, because in the most SMAs, the amount of volumetric strain during martensitic transformation is small (around 0.003), but for $Ti_{50}Pd_{40}Ni_{10}$ HTSMA, the volumetric strain is higher (around 0.0104). This higher volumetric strain of $Ti_{50}Pd_{40}Ni_{10}$ and also lower resistance to plastic

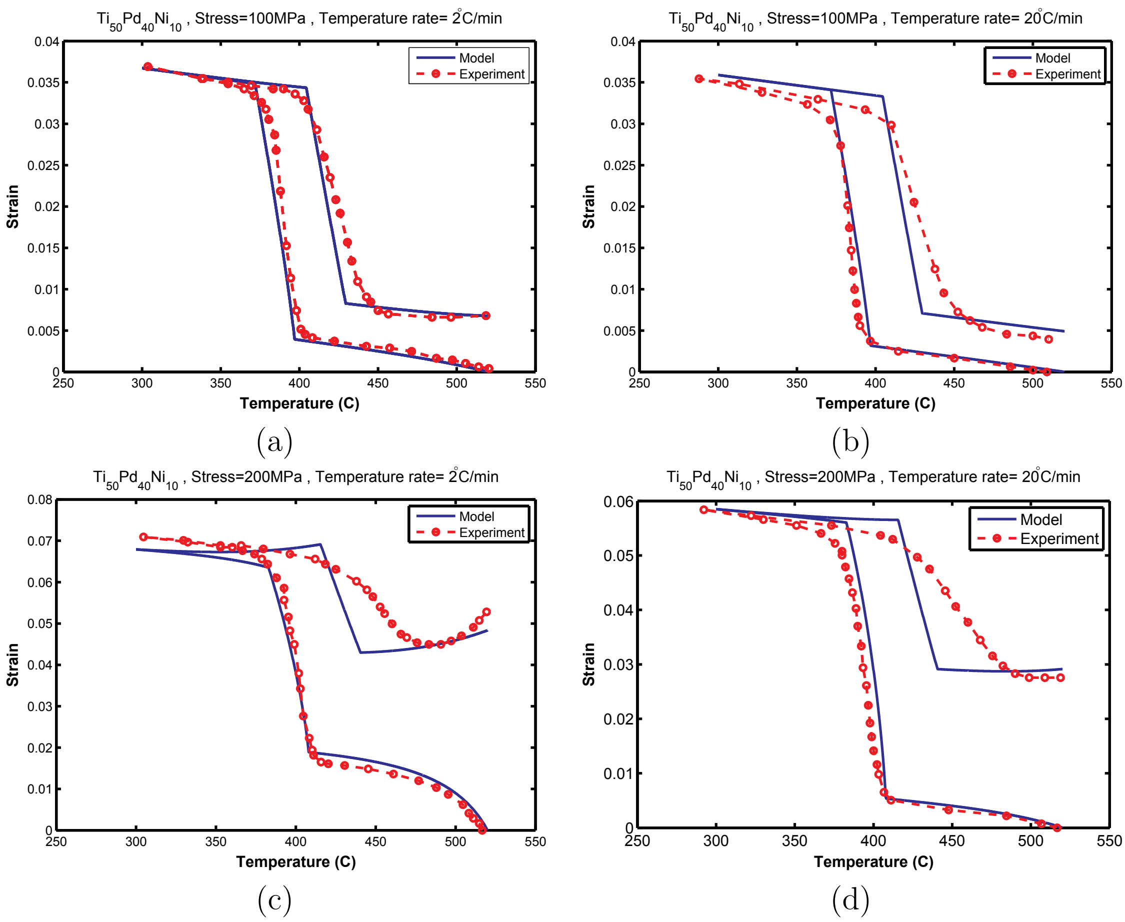


Figure 6: Comparison of 1D simulation and experiments for strain-temperature behavior of the $Ti_{50}Pd_{40}Ni_{10}$ specimen thermally cycled at (a) $2°C/min$ under 100MPa applied stress, (b)$20°C/min$ under 100MPa , (c)$2°C/min$ under 200MPa and (d) $20°C/min$ under 200MPa

deformation in this alloy may be due to the existence of Pd atoms which affect the martensitic transformation and the material properties, making $Ti_{50}Pd_{40}Ni_{10}$ more vulnerable to the transformation induced plasticity.

5 CONCLUSION

In this study, an investigation on the effects of martensite plates in the austenitic phase during the martensitic transformation in shape memory alloys is presented. The different factors which affect the internal stress field of the microstructure were illustrated. To model the coexistence of plastic strain and martensitic transformation in high temperature shape memory alloys, the phenomenological constitutive equations are presented to simulate the macroscopic behavior of high temperature shape memory alloys based on the effective parameters on the internal stress field. The comparison between the results of simulation and experiments verify the applicability of the model for one dimensional uni axial loadings.

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